PCA - An example on Exploratory Data Analysis

In this notebook you will:

- Replicate Andrew's example on PCA
- Visualize how PCA works on a 2-dimensional small dataset and that not every projection is "good"
- Visualize how a 3-dimensional data can also be contained in a 2-dimensional subspace
- Use PCA to find hidden patterns in a high-dimensional dataset

Importing the libraries

In [1]:
```
import pandas as pd
import numpy as np
from sklearn.decomposition import PCA
from pca_utils import plot_widget
from bokeh.io import show, output_notebook
from bokeh.plotting import figure
import matplotlib.pyplot as plt
import plotly.offline as py
```

In [2]:
```
py.init_notebook_mode()
```

In [3]:
```
output_notebook()
```

BokehJS 2.4.3 successfully loaded.

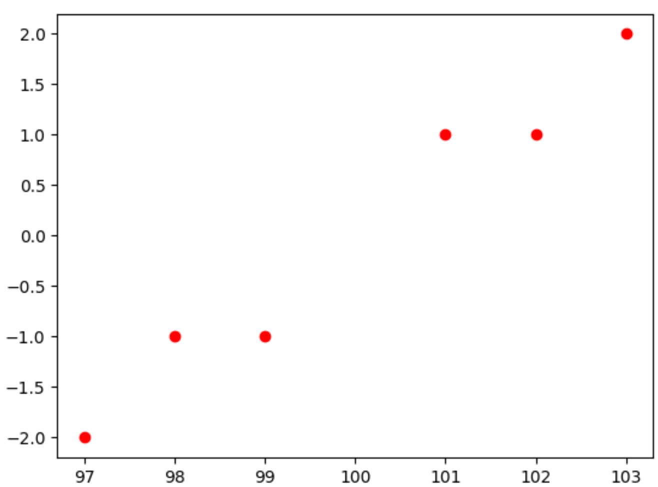
Lecture Example

We are going work on the same example that Andrew has shown in the lecture.

In [4]:
```
X = np.array([[ 99,  -1],
       [ 98,  -1],
       [ 97,  -2],
       [101,   1],
       [102,   1],
       [103,   2]])
```

In [5]:
```
plt.plot(X[:,0], X[:,1], 'ro')
```

Out[5]:
```
[<matplotlib.lines.Line2D at 0x7d0dd4f88ad0>]
```



In [6]:
```
# Loading the PCA algorithm
pca_2 = PCA(n_components=2)
pca_2
```

Out[6]:
```
PCA(n_components=2)
```

In [7]:
```
# Let's fit the data. We do not need to scale it, since sklearn's implementation already handles it.
pca_2.fit(X)
```

Out[7]:
```
PCA(n_components=2)
```

In [8]:
```
pca_2.explained_variance_ratio_
```

Out[8]:
```
array([0.99244289, 0.00755711])
```

The coordinates on the first principal component (first axis) are enough to retain 99.24% of the information ("explained variance"). The second principal component adds an additional 0.76% of the information ("explained variance") that is not stored in the first principal component coordinates.

In [9]:
```
X_trans_2 = pca_2.transform(X)
X_trans_2
```

Out[9]:
```
array([[ 1.38340578,  0.2935787 ],
       [ 2.22189802, -0.25133484],
       [ 3.6053038 ,  0.04224385],
       [-1.38340578, -0.2935787 ],
       [-2.22189802,  0.25133484],
       [-3.6053038 , -0.04224385]])
```

Think of column 1 as the coordinate along the first principal component (the first new axis) and column 2 as the coordinate along the second principal component (the second new axis).

You can probably just choose the first principal component since it retains 99% of the information (explained variance).

In [10]:
```
pca_1 = PCA(n_components=1)
pca_1
```

Out[10]:
```
PCA(n_components=1)
```

In [11]:
```
pca_1.fit(X)
pca_1.explained_variance_ratio_
```

Out[11]:
```
array([0.99244289])
```

In [12]:
```
X_trans_1 = pca_1.transform(X)
X_trans_1
```

Out[12]:
```
array([[ 1.38340578],
       [ 2.22189802],
       [ 3.6053038 ],
       [-1.38340578],
       [-2.22189802],
       [-3.6053038 ]])
```

Notice how this column is just the first column of `X_trans_2`.

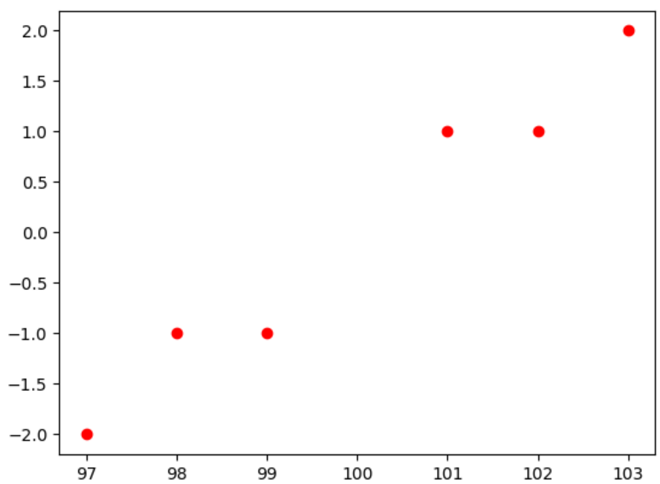
If you had 2 features (two columns of data) and choose 2 principal components, then you'll keep all the information and the data will end up the same as the original.

In [13]:
```
X_reduced_2 = pca_2.inverse_transform(X_trans_2)
X_reduced_2
```

Out[13]:
```
array([[ 99.,  -1.],
       [ 98.,  -1.],
       [ 97.,  -2.],
       [101.,   1.],
       [102.,   1.],
       [103.,   2.]])
```

In [14]:
```
plt.plot(X_reduced_2[:,0], X_reduced_2[:,1], 'ro')
```

Out[14]:
```
[<matplotlib.lines.Line2D at 0x7d0dd4666150>]
```



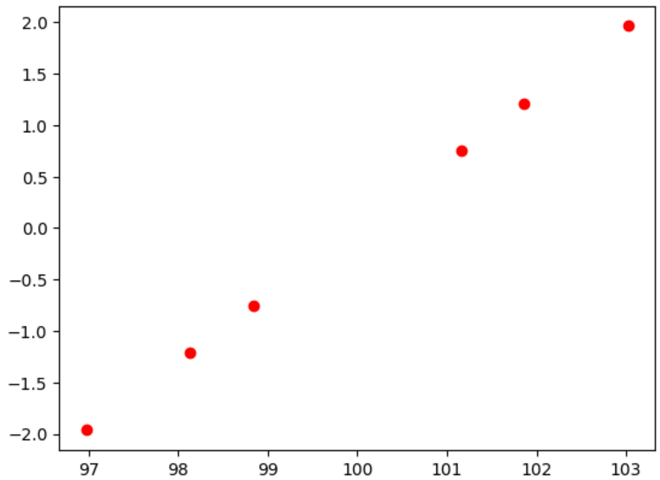
Reduce to 1 dimension instead of 2

In [15]:
```
X_reduced_1 = pca_1.inverse_transform(X_trans_1)
X_reduced_1
```

Out[15]:
```
array([[ 98.84002499,  -0.75383654],
       [ 98.13695576,  -1.21074232],
       [ 96.97698075,  -1.96457886],
       [101.15997501,   0.75383654],
       [101.86304424,   1.21074232],
       [103.02301925,   1.96457886]])
```

In [16]:
```
plt.plot(X_reduced_1[:,0], X_reduced_1[:,1], 'ro')
```

Out[16]:
```
[<matplotlib.lines.Line2D at 0x7d0dd45d77d0>]
```



Notice how the data are now just on a single line (this line is the single principal component that was used to describe the data; and each example had a single "coordinate" along that axis to describe its location.

Visualizing the PCA algorithm

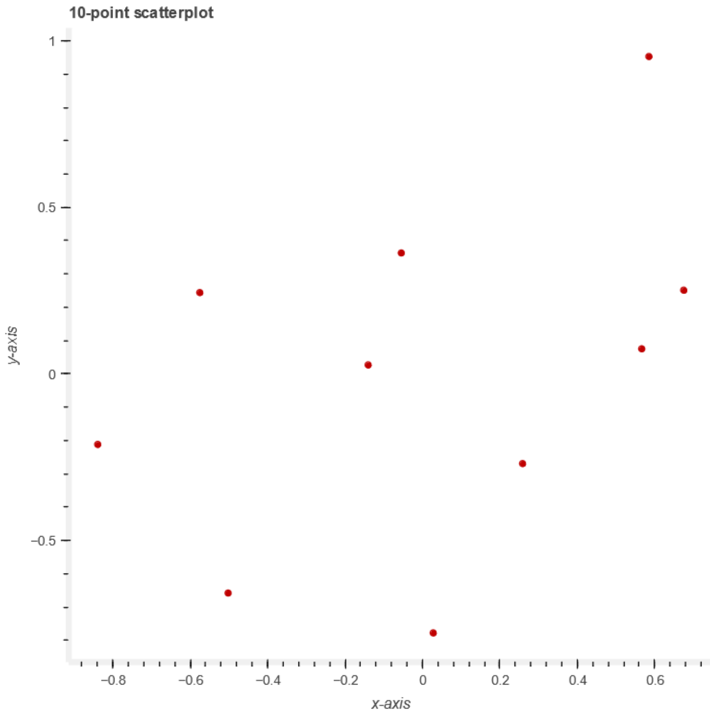
Let's define 10 points in the plane and use them as an example to visualize how we can compress this points in 1 dimension. You will see that there are good ways and bad ways.

In [17]:
```
X = np.array([[-0.83934975, -0.21160323],
       [ 0.67508491,  0.25113527],
       [-0.05495253,  0.36339613],
       [-0.57524042,  0.24450324],
       [ 0.58468572,  0.95337657],
       [ 0.5663363 ,  0.07555096],
       [-0.50228538, -0.65749982],
       [-0.14075593,  0.02713815],
       [ 0.2587186 , -0.26890678],
       [ 0.02775847, -0.77709049]])
```

In [18]:
```
p = figure(title = '10-point scatterplot', x_axis_label = 'x-axis', y_axis_label = 'y-axis') ## Creates the figure object
p.scatter(X[:,0],X[:,1],marker = 'o', color = '#C00000', size = 5) ## Add the scatter plot

## Some visual adjustments
p.grid.visible = False
p.grid.visible = False
p.outline_line_color = None
p.toolbar.logo = None
p.toolbar_location = None
p.xaxis.axis_line_color = "#f0f0f0"
p.xaxis.axis_line_width = 5
p.yaxis.axis_line_color = "#f0f0f0"
p.yaxis.axis_line_width = 5

## Shows the figure
show(p)
```



The next code will generate a widget where you can see how different ways of compressing this data into 1-dimensional datapoints will lead to different ways on how the points are spread in this new space. The line generated by PCA is the line that keeps the points as far as possible from each other.

You can use the slider to rotate the black line through its center and see how the points' projection onto the line will change as we rotate the line.

You can notice that there are projections that place different points in almost the same point, and there are projections that keep the points as separated as they were in the plane.

In [19]:
```
plot_widget()
```

```
HBox(children=(FigureWidget({
    'data': [{'hovertemplate': 'x=%{x}<br>y=%{y}<extra></extra>',
            …
```

Visualization of a 3-dimensional dataset

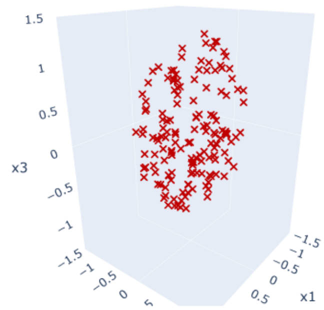
In this section we will see how some 3 dimensional data can be condensed into a 2 dimensional space.

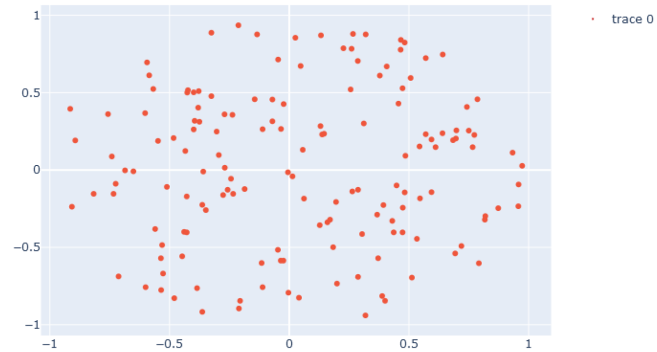
In [20]:
```
from pca_utils import random_point_circle, plot_3d_2d_graphs
```

In [21]:
```
X = random_point_circle(n = 150)
```

In [22]:
```
deb = plot_3d_2d_graphs(X)
```

In [23]:
```
deb.update_layout(yaxis2 = dict(title_text = 'test', visible=True))
```





Using PCA in Exploratory Data Analysis

Let's load a toy dataset with 500 samples and 1000 features.

In [24]:
```
df = pd.read_csv("toy_dataset.csv")
```

In [25]:
```
df.head()
```

Out[25]:

	feature_0	feature_1	feature_2	feature_3	feature_4	feature_5	feature_6	feature_7	feature_8	feature_9	...	feature_990	feature_991	feature_992	feature_993	fea
0	27.422157	-29.662712	-23.297163	-15.161935	0.345581	3.706750	-5.507209	-46.992476	5.175469	-47.768145	...	7.815960	24.320965	-33.987522	22.306088	3
1	3.489482	-19.153551	-14.636424	14.688258	20.114204	13.532852	34.298084	22.982509	37.938670	-35.648144	...	11.145527	-38.886603	44.579337	37.308519	2
2	4.293509	22.691579	-1.045155	-8.740350	12.401082	31.362987	-18.831206	-35.384557	8.161430	-16.421762	...	48.190331	-0.503157	-21.740678	15.972237	
3	-2.139348	23.158754	-26.241206	19.426465	9.472049	8.453948	0.637211	-26.675984	-43.823329	11.840874	...	-51.613076	13.278858	-44.179281	32.912282	
4	-35.251034	27.281816	-29.470282	-21.786865	11.806822	58.655133	5.375230	59.740676	-49.007717	-21.801155	...	0.010857	20.975655	-21.358371	18.709369	2

5 rows × 1000 columns

This is a dataset with 1000 features.

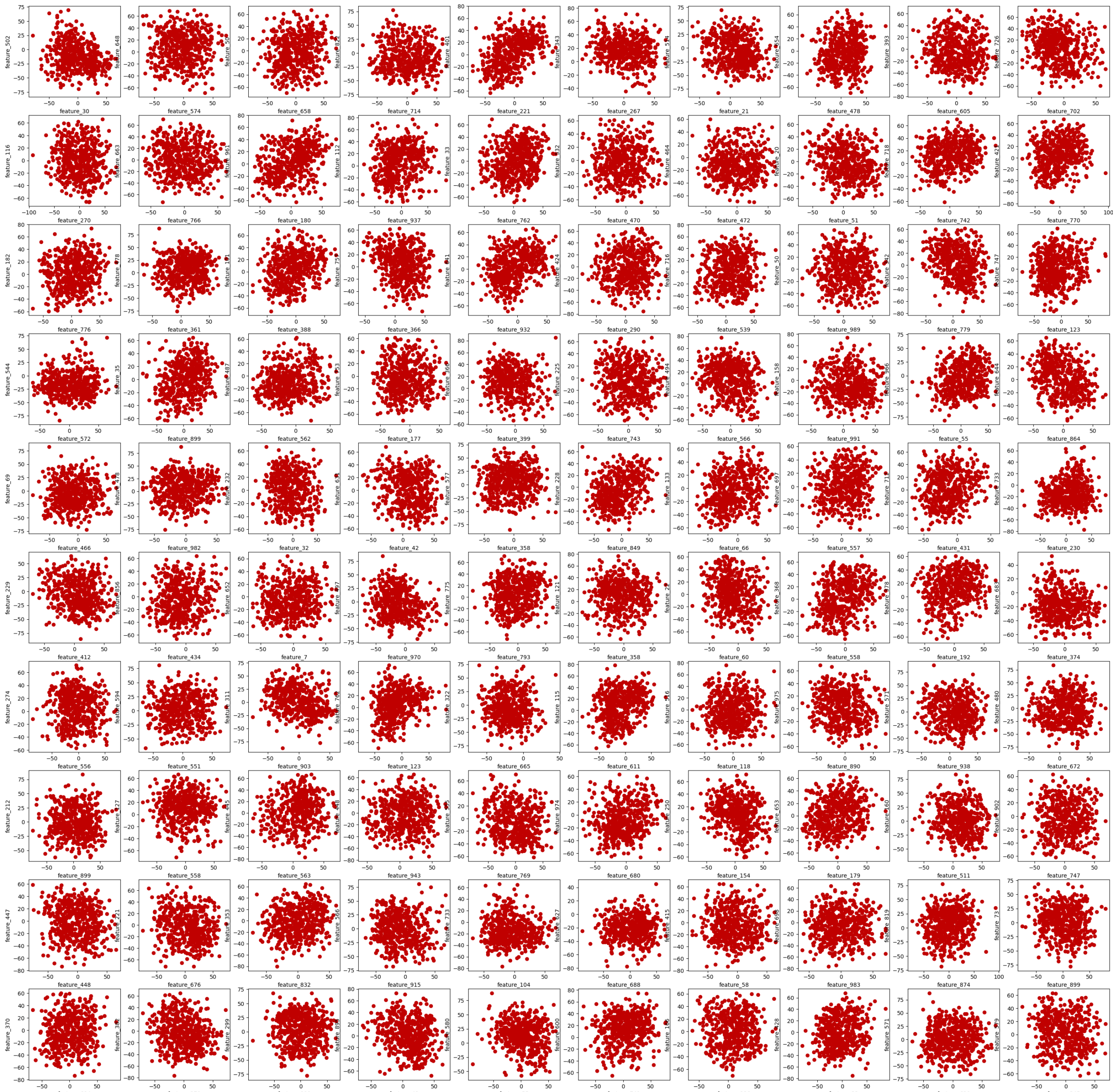
Let's try to see if there is a pattern in the data. The following function will randomly sample 100 pairwise tuples (x,y) of features, so we can scatter-plot them.

In [26]:
```
def get_pairs(n = 100):
    from random import randint
    i = 0
    tuples = []
    while i < 100:
        x = df.columns[randint(0,999)]
        y = df.columns[randint(0,999)]
        while x == y or (x,y) in tuples or (y,x) in tuples:
            y = df.columns[randint(0,999)]
        tuples.append((x,y))
        i+=1
    return tuples
```

In [27]:
```
pairs = get_pairs()
```

Now let's plot them!

In [28]:
```
fig, axs = plt.subplots(10,10, figsize = (35,35))
i = 0
for rows in axs:
    for ax in rows:
        ax.scatter(df[pairs[i][0]],df[pairs[i][1]], color = "#C00000")
        ax.set_xlabel(pairs[i][0])
        ax.set_ylabel(pairs[i][1])
        i+=1
```



It looks like there is not much information hidden in pairwise features. Also, it is not possible to check every combination, due to the amount of features. Let's try to see the linear correlation between them.

In [29]:
```
# This may take 1 minute to run
corr = df.corr()
```

In [30]:
```
## This will show all the features that have correlation > 0.5 in absolute value. We remove the features
## with correlation == 1 to remove the correlation of a feature with itself

mask = (abs(corr) > 0.5) & (abs(corr) != 1)
corr.where(mask).stack().sort_values()
```

Out[30]:
```
feature_81   feature_657   -0.631294
feature_657  feature_81    -0.631294
feature_313  feature_4     -0.615317
feature_4    feature_313   -0.615317
feature_716  feature_1     -0.609056
                              ...
feature_792  feature_547    0.620864
feature_35   feature_965    0.631424
feature_965  feature_35     0.631424
feature_395  feature_985    0.632593
feature_985  feature_395    0.632593
Length: 1870, dtype: float64
```

The maximum and minimum correlation is around 0.631 - 0.632. This does not show too much as well.

Let's try PCA decomposition to compress our data into a 2-dimensional subspace (plane) so we can plot it as scatter plot.

In [31]:
```
# Loading the PCA object
pca = PCA(n_components = 2) # Here we choose the number of components that we will keep.
X_pca = pca.fit_transform(df)
df_pca = pd.DataFrame(X_pca, columns = ['principal_component_1','principal_component_2'])
```

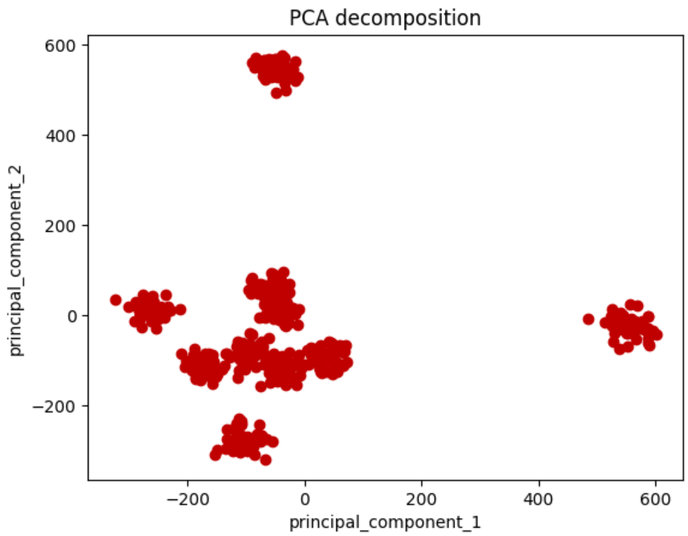
In [32]:
```
df_pca.head()
```

Out[32]:

	principal_component_1	principal_component_2
0	-46.235641	-1.672797
1	-210.208758	-84.068249
2	-26.352795	-127.895751
3	-116.106804	-269.368256
4	-110.183605	-279.657306

In [33]:
```
plt.scatter(df_pca['principal_component_1'],df_pca['principal_component_2'], color = "#C00000")
plt.xlabel('principal_component_1')
plt.ylabel('principal_component_2')
plt.title('PCA decomposition')
```

Out[33]:
```
Text(0.5, 1.0, 'PCA decomposition')
```



This is great! We can see well defined clusters.

In [34]:
```
# pca.explained_variance_ration_ returns a list where it shows the amount of variance explained by each principal component.
sum(pca.explained_variance_ratio_)
```

Out[34]:
```
0.1457284355510628
```

And we preserved only around 14.6% of the variance!

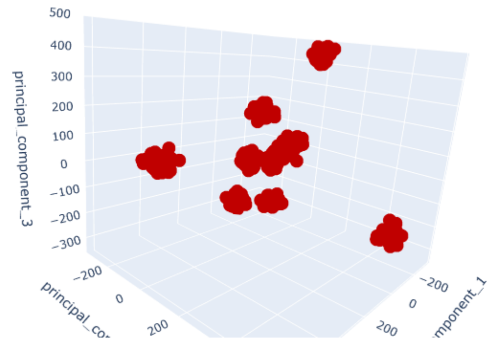
Quite impressive! We can clearly see clusters in our data, something that we could not see before. How many clusters can you spot? 8, 10?

If we run a PCA to plot 3 dimensions, we will get more information from data.

In [35]:
```
pca_3 = PCA(n_components = 3).fit(df)
X_t = pca_3.transform(df)
df_pca_3 = pd.DataFrame(X_t,columns = ['principal_component_1','principal_component_2','principal_component_3'])
```

In [36]:
```
import plotly.express as px
```

In [37]:
```
fig = px.scatter_3d(df_pca_3, x = 'principal_component_1', y = 'principal_component_2', z = 'principal_component_3').update_traces(marker = dict(color
fig.show()
```




```
In [38]: sum(pca_3.explained_variance_ratio_)
```

Out[38]: 0.2080625781609324

Now we preserved 19% of the variance and we can clearly see 10 clusters.

Congratulations on finishing this notebook!